

07/07/2005 10726183.trn

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07/07/2005 10726183.trn

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NEWS WWW CAS World Wide Web Site (general information)

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FILE 'HOME' ENTERED AT 13:12:05 ON 07 JUL 2005

=> FIL REGISTRY  
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 13:12:25 ON 07 JUL 2005  
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STRUCTURE FILE UPDATES: 6 JUL 2005 HIGHEST RN 853990-77-9  
DICTIONARY FILE UPDATES: 6 JUL 2005 HIGHEST RN 853990-77-9

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**TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005**

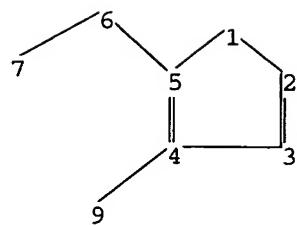
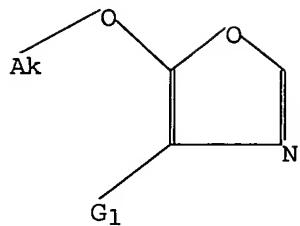
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*****
* The CA roles and document type information have been removed from
* the IDE default display format and the ED field has been added,
* effective March 20, 2005. A new display format, IDERL, is now
* available and contains the CA role and document type information.
*  
*****
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10726183.str



chain nodes :

6 7 9

ring nodes :

1 2 3 4 5

chain bonds :

4-9 5-6 6-7

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

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exact bonds :

1-2 1-5 4-5

isolated ring systems :

containing 1 :

G1:H,Ak

Match level :

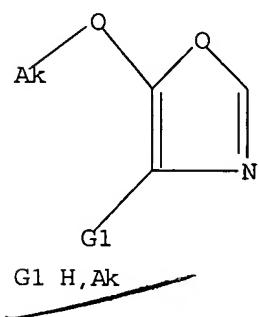
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 9:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 13:12:39 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 169 TO ITERATE

100.0% PROCESSED 169 ITERATIONS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 2601 TO 4159  
 PROJECTED ANSWERS: 640 TO 1520

L2 50 SEA SSS SAM L1

=> S 11 SSS full  
 FULL SEARCH INITIATED 13:12:46 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 3219 TO ITERATE

100.0% PROCESSED 3219 ITERATIONS  
 SEARCH TIME: 00.00.01

1024 ANSWERS

L3 1024 SEA SSS FUL L1

=> FIL CAPLUS  
~~COST IN U.S. DOLLARS~~  
 FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
161.33	161.54

FILE 'CAPLUS' ENTERED AT 13:13:00 ON 07 JUL 2005  
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 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE COVERS 1907 - 7 Jul 2005 VOL 143 ISS 2  
 FILE LAST UPDATED: 6 Jul 2005 (20050706/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> S 13  
 L4 426 L3

=> S 14 and isocyanoalkanoate  
 6 ISOCYANOALKANOATE  
 10 ISOCYANOALKANOATES  
 13 ISOCYANOALKANOATE  
 (ISOCYANOALKANOATE OR ISOCYANOALKANOATES)  
 3 L4 AND ISOCYANOALKANOATE

07/07/2005 10726183.trn

=> s 13/p  
L6 274 L3/P

=> s 16 and continuously  
L7 137715 CONTINUOUSLY  
2 L6 AND CONTINUOUSLY

=> s 16 and isocyano  
L8 1075 ISOCYANO  
7 L6 AND ISOCYANO

=> s 16 and isocyanoalkanoate  
6 ISOCYANOALKANOATE  
10 ISOCYANOALKANOATES  
13 ISOCYANOALKANOATE  
(ISOCYANOALKANOATE OR ISOCYANOALKANOATES)  
L9 3 L6 AND ISOCYANOALKANOATE

=> s 16 and p/dt  
4742472 P/DT  
L10 101 L6 AND P/DT

=> s 110 us/pc  
MISSING OPERATOR L10 US/PC  
The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s 110 pc/us  
MISSING OPERATOR L10 PC/US  
The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s 110 and pc/us  
'US' IS NOT A VALID FIELD CODE  
0 PC/US  
L11 0 L10 AND PC/US

=> s 110 and us/pc  
1386329 US/PC  
L12 50 L10 AND US/PC

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20650021 PY<=2000  
L13 30 L12 AND PY<=2000

=> d his

(FILE 'HOME' ENTERED AT 13:12:05 ON 07 JUL 2005)

FILE 'REGISTRY' ENTERED AT 13:12:25 ON 07 JUL 2005  
L1 STRUCTURE uploaded  
L2 50 S L1  
L3 1024 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 13:13:00 ON 07 JUL 2005  
L4 426 S L3  
L5 3 S L4 AND ISOCYANOALKANOATE  
L6 274 S L3/P

L7        2 S L6 AND CONTINUOUSLY  
L8        7 S L6 AND ISOCYANO  
L9        3 S L6 AND ISOCYANOALKANOATE  
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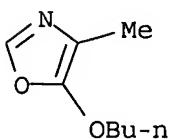
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L5        ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2003:512125 CAPLUS  
DOCUMENT NUMBER: 139:86982  
TITLE: Process for the preparation of substituted oxazoles  
INVENTOR(S): Rust, Harald; Burkart, Kirsten; Faust, Tillmann;  
                 Henkelmann, Jochem; Kindler, Alois; Knoll, Christian;  
                 Becker, Michael  
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany  
SOURCE: U.S. Pat. Appl. Publ., 11 pp., Cont.-in-part of U.S.  
                 Ser. No. 209,529.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

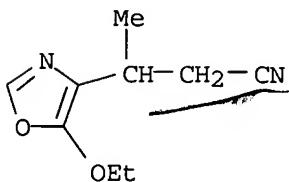
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003125567	A1	20030703	US 2003-348961	20030123
US 6900332	B2	20050531		
DE 10137480	A1	20030213	DE 2001-10137480	20010803
DE 10209446	A1	20030918	DE 2002-10209446	20020305
US 2003050479	A1	20030313	US 2002-209529	20020801
JP 2003176272	A2	20030624	JP 2002-227292	20020805
JP 2003267958	A2	20030925	JP 2002-355822	20021206
CN 1442412	A	20030917	CN 2002-156818	20021213
PRIORITY APPLN. INFO.:			DE 2001-10137480	A 20010803
			DE 2002-10209446	A 20020305
			US 2002-209529	A2 20020801

OTHER SOURCE(S): MARPAT 139:86982

- AB The present invention relates to a process for preparing 5-alkoxy-substituted oxazoles, in particular for preparing 4-methyl-5-alkoxy-substituted oxazoles and also a process for preparing pyridoxine derivs. The process is carried out in a batchwise or semibatchwise reactor equipped with an emplaced reaction column and, simultaneously with the conversion, removing the 5-alkoxy-substituted oxazoles from the reaction mixture by rectification provided that the parameters of the rectification are set in such a way that the  $\alpha$ - isocyanooalkanoate esters are converted to the 5-alkoxy-substituted oxazoles in the reactor and/or on the internals of the emplaced reaction column and the 5-alkoxy-substituted oxazoles resulting from the conversion are removed via the emplaced reaction column.
- IT 24201-52-3P, 5-Butoxy-4-methyloxazole  
RL: IMF (Industrial manufacture); PREP (Preparation)  
                 (batchwise or semibatchwise process for preparation of substituted oxazoles)
- RN 24201-52-3 CAPLUS  
CN Oxazole, 5-butoxy-4-methyl- (8CI, 9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1974:27047 CAPLUS  
 DOCUMENT NUMBER: 80:27047  
 TITLE: Synthesis with  $\alpha$ -metalated isocyanides. XXV.  
 Ethyl 4-cyano-2-isocyanoalkanoates, ethyl  
 4-cyano-2-(formylamino)alkanoates, and ethyl  
 4-cyano-5(4)-pyrroline-2-carboxylate from  
 $\alpha$ -metalated ethyl isocyanoalkanoates  
 and acrylonitriles  
 AUTHOR(S): Schoellkopf, Ulrich; Porsch, Paul H.  
 CORPORATE SOURCE: Org.-Chem. Inst., Univ. Goettingen, Goettingen, Fed.  
 Rep. Ger.  
 SOURCE: Chemische Berichte (1973), 106(10), 3382-90  
 CODEN: CHBEAM; ISSN: 0009-2940  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 GI For diagram(s), see printed CA Issue.  
 AB EtO<sub>2</sub>CCR(NC)CHR<sub>1</sub>CHR<sub>2</sub>CN (R, R<sub>2</sub> = H, Me; R<sub>1</sub> = H, Me, Ph) and  
 EtO<sub>2</sub>CC(NC)(CHR<sub>1</sub>CHR<sub>2</sub>CN)<sub>2</sub> were prepared by reaction of R<sub>1</sub>CH:CR<sub>2</sub>CN (I) with  
 EtO<sub>2</sub>CCHRN<sub>C</sub> (II) in EtOH at .apprx.30° in the presence of catalytic  
 amts. EtONa. By treating with aqueous HCl, the isocyano group of the compds.  
 obtained was converted into the formylamino group. Reaction of I with II  
 in EtOH at .apprx.65° in the presence of equivalent amts. EtONa yielded  
 in the case of R<sub>2</sub> = Me the pyrrolines III and in the case of R<sub>2</sub> = H the  
 pyrrolines IV.  
 IT 51068-91-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 51068-91-8 CAPLUS  
 CN 4-Oxazolepropanenitrile, 5-ethoxy- $\beta$ -methyl- (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1971:448961 CAPLUS  
 DOCUMENT NUMBER: 75:48961  
 TITLE: Synthetic intermediate of pyridoxine. II. Thermal  
 cyclization of ethyl  $\alpha$ -isocyano propionate to  
5-ethoxy-4-methyloxazole  
 AUTHOR(S): Maeda, Itsutoshi; Togo, Kazushi; Yoshida, Ryonosuke  
 CORPORATE SOURCE: Cent. Res. Lab., Ajinomoto Co., Inc., Kawasaki, Japan  
 SOURCE: Bulletin of the Chemical Society of Japan (1971),  
 44(5), 1407-10

CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal  
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The thermal cyclization of ethyl  $\alpha$ -isocyanopropionate (I) gave 5-ethoxy-4-methyloxazole (II) as an intermediate for the synthesis of pyridoxine. The similar reaction of several alkyl esters of  $\alpha$ -isocyanocarboxylic acid to the corresponding 5-alkoxy-4-substituted oxazole was also carried out. The products of the thermal cyclization of I were investigated. When the cyclization was carried out 5 hr at 180°, the maximum yield of the main product, II, was 20%; unreacted I (30%), Et  $\alpha$ -cyanopropionate (20%), and dimer of I (5%) were also obtained. The  $\alpha$ -H of Et  $\alpha$ -isocyanosuccinate (III) can be more easily removed than that of I, so III may be expected to be more readily converted to 5-ethoxy-4-ethoxycarbonylmethyloxazole (IV), which is also an intermediate of pyridoxine. The yield of IV from III was <30% because of the side reaction.

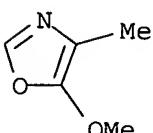
IT 1622-76-0P 5006-20-2P 5214-69-7P

15031-12-6P 24201-52-3P 33115-82-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

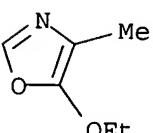
RN 1622-76-0 CAPIUS

CN Oxazole, 5-methoxy-4-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



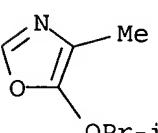
RN 5006-20-2 CAPIUS

CN Oxazole, 5-ethoxy-4-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



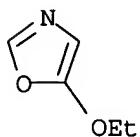
RN 5214-69-7 CAPIUS

CN Oxazole, 4-methyl-5-(1-methylethoxy)- (9CI) (CA INDEX NAME)

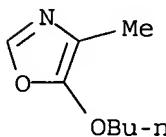


RN 15031-12-6 CAPIUS

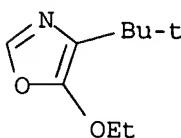
CN Oxazole, 5-ethoxy- (8CI, 9CI) (CA INDEX NAME)



RN 24201-52-3 CAPLUS  
 CN Oxazole, 5-butoxy-4-methyl- (8CI, 9CI) (CA INDEX NAME)



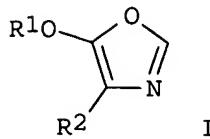
RN 33115-82-1 CAPLUS  
 CN Oxazole, 5-ethoxy-4-isobutyl- (8CI) (CA INDEX NAME)



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L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2004:649326 CAPLUS  
 DOCUMENT NUMBER: 141:174164  
 TITLE: Preparation of 5-alkoxyoxazoles from isocyano esters  
       in the presence of tertiary amines.  
 INVENTOR(S): Arndt, Jan-dirk; Henkelmann, Jochem; Burkart, Kirsten;  
                 Heimann, Frank; Rust, Harald; Becker, Michael  
 PATENT ASSIGNEE(S): BASF Ag, Germany  
 SOURCE: Ger. Offen., 15 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10304343	A1	20040812	DE 2003-10304343	20030203
PRIORITY APPLN. INFO.:			DE 2003-10304343	20030203
OTHER SOURCE(S):	CASREACT	141:174164; MARPAT 141:174164		
GI				



AB Title compds. [I; R1 = (substituted) alkyl; R2 = H, (substituted) alkyl], were prepared by heating CNCHR<sub>2</sub>CO<sub>2</sub>R<sub>1</sub> (variables as above) at >80° with NR<sub>5</sub>R<sub>6</sub>R<sub>7</sub> [R<sub>5</sub>-R<sub>7</sub> = (substituted) alkyl, cycloalkyl; NR<sub>5</sub>R<sub>6</sub> = atoms to form a 3-7 membered (unsatd.) heterocycl; the mol. weight of NR<sub>5</sub>R<sub>6</sub>R<sub>7</sub> is >185]. Thus, a mixture of CNCHMeCO<sub>2</sub>Bu, dibutylpentylamine, PhMe, BuOH, and traces of N-formylalanine Bu ester was reacted continuously at 170° through a 3-step stirred vessel cascade with a retention time of 25 min. per vessel to give a 41% yield of 4-methyl-5-butoxyoxazole at 50% conversion. A process for prepn of pyridoxine derivs. from I and protected butenediols is claimed.

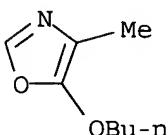
IT 24201-52-3P, 5-Butoxy-4-methyloxazole

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of alkoxyoxazoles from isocyano esters in the presence of tertiary amines)

RN 24201-52-3 CAPLUS

CN Oxazole, 5-butoxy-4-methyl- (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:492747 CAPLUS

DOCUMENT NUMBER: 139:70706

TITLE: Continuous preparation of 5-alkoxy-substituted oxazoles

INVENTOR(S): Rust, Harald; Burkart, Kirsten; Faust, Tillmann; Henkelmann, Jochem; Knoll, Christian; Mohry, Andre; Kindler, Alois

PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany

SOURCE: U.S. Pat. Appl. Publ., 11 pp., Cont.-in-part of U.S. Ser. No. 207,894.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003120082	A1	20030626	US 2002-300629	20021121
US 6713630	B2	20040330		
DE 10137627	A1	20030220	DE 2001-10137627	20010803
DE 10209447	A1	20030918	DE 2002-10209447	20020305

US 2003050478	A1	20030313	US 2002-207894	20020731
JP 2003201283	A2	20030718	JP 2002-227742	20020805
JP 2003261546	A2	20030919	JP 2002-355604	20021206
CN 1442411	A	20030917	CN 2002-156817	20021213
US 2004110961	A1	20040610	US 2003-726183	20031203
PRIORITY APPLN. INFO.:				
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			US 2002-300629	A3 20021121

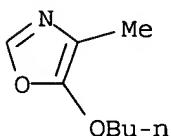
OTHER SOURCE(S): CASREACT 139:70706; MARPAT 139:70706

AB The present invention relates to a process for **continuously** preparing 5-alkoxy-substituted oxazoles, in particular for **continuously** preparing 4-methyl-5-alkoxy-substituted oxazoles and also a process for preparing pyridoxine derivs. Thus, 4-methyl-5-n-butoxyoxazole was synthesized from n-Bu  $\alpha$ -isocyanopropionate in the presence of tri-n-butylamine.

IT 24201-52-3P, 4-Methyl-5-n-butoxyoxazole  
 RL: CPS (Chemical process); IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); PROC (Process); USES (Uses)  
 (continuous preparation of 5-alkoxy-substituted oxazoles)

RN 24201-52-3 CAPLUS

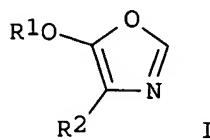
CN Oxazole, 5-butoxy-4-methyl- (8CI, 9CI) (CA INDEX NAME)



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L8 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2004:649326 CAPLUS  
 DOCUMENT NUMBER: 141:174164  
 TITLE: Preparation of 5-alkoxyoxazoles from **isocyano** esters in the presence of tertiary amines.  
 INVENTOR(S): Arndt, Jan-dirk; Henkelmann, Jochem; Burkart, Kirsten; Heimann, Frank; Rust, Harald; Becker, Michael  
 PATENT ASSIGNEE(S): BASF Ag, Germany  
 SOURCE: Ger. Offen., 15 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10304343	A1	<del>20040612</del>	DE 2003-10304343	20030203
PRIORITY APPLN. INFO.:				
OTHER SOURCE(S): CASREACT 141:174164; MARPAT 141:174164				
GI				



AB Title compds. [I; R1 = (substituted) alkyl; R2 = H, (substituted) alkyl], were prepared by heating CNCHR<sub>2</sub>CO<sub>2</sub>R<sub>1</sub> (variables as above) at >80° with NR<sub>5</sub>R<sub>6</sub>R<sub>7</sub> [R<sub>5</sub>-R<sub>7</sub> = (substituted) alkyl, cycloalkyl; NR<sub>5</sub>R<sub>6</sub> = atoms to form a 3-7 membered (unsatd.) heterocyclol; the mol. weight of NR<sub>5</sub>R<sub>6</sub>R<sub>7</sub> is >185]. Thus, a mixture of CNCHMeCO<sub>2</sub>Bu, dibutylpentylamine, PhMe, BuOH, and traces of N-formylalanine Bu ester was reacted continuously at 170° through a 3-step stirred vessel cascade with a retention time of 25 min. per vessel to give a 41% yield of 4-methyl-5-butoxyoxazole at 50% conversion. A process for prepn of pyridoxine derivs. from I and protected butenediols is claimed.

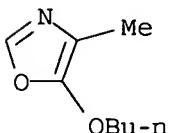
IT 24201-52-3P, 5-Butoxy-4-methyloxazole

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of alkoxyoxazoles from **isocyano** esters in the presence of tertiary amines)

RN 24201-52-3 CAPLUS

CN Oxazole, 5-butoxy-4-methyl- (8CI, 9CI) (CA INDEX NAME)



L8 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:515403 CAPLUS

DOCUMENT NUMBER: 113:115403

TITLE: Synthesis and aldol-type reaction of 5-methoxy-2-(trialkylsilyl)oxazoles

AUTHOR(S): Murakami, Masahiro; Higuchi, Noriko; Ito, Yoshihiko

CORPORATE SOURCE: Fac. Eng., Kyoto Univ., Yoshida, 606, Japan

SOURCE: Chemistry Express (1990) 5(6), 411-14

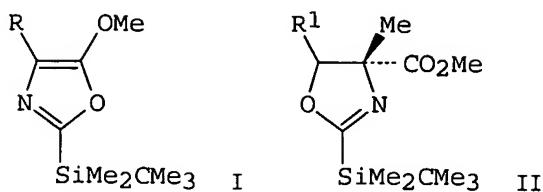
CODEN: CHEXEU; ISSN: 0911-9566

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:115403

GI

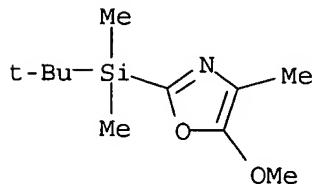


AB Lithiation of  $\alpha$ - **isocyno** carboxylic esters  $\text{MeO}_2\text{CCH}(\text{NC})\text{R}$  followed by silylation with trialkylchlorosilane afforded methoxy(trialkylsilyl)oxazoles (I; R = Me, Et, CMe<sub>2</sub>). I (R = Me) underwent  $\text{ZnCl}_2$ -catalyzed aldol-type condensation with R<sub>1</sub>CHO (R<sub>1</sub> = alkyl, Ph) to produce *cis* and *trans* isomers of (methoxycarbonyl)(trialkylsilyl)oxazolines (II; R<sub>1</sub> = alkyl, Ph).

IT 129206-70-8P 129206-71-9P 129206-72-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and aldol condensation of, oxazoline derivs. by)

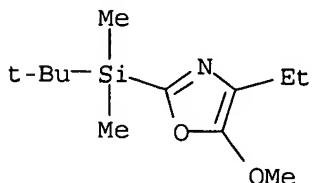
RN 129206-70-8 CAPLUS

CN Oxazole, 2-[(1,1-dimethylethyl)dimethylsilyl]-5-methoxy-4-methyl- (9CI)  
 (CA INDEX NAME)



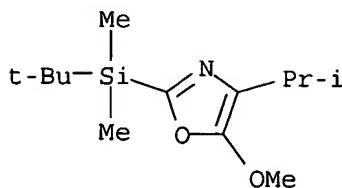
RN 129206-71-9 CAPLUS

CN Oxazole, 2-[(1,1-dimethylethyl)dimethylsilyl]-4-ethyl-5-methoxy- (9CI)  
 (CA INDEX NAME)

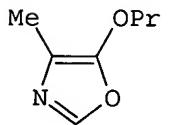


RN 129206-72-0 CAPLUS

CN Oxazole, 2-[(1,1-dimethylethyl)dimethylsilyl]-5-methoxy-4-(1-methylethyl)- (9CI) (CA INDEX NAME)

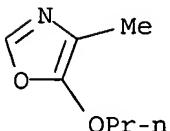


L8 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1989:114729 CAPLUS  
 DOCUMENT NUMBER: 110:114729  
 TITLE: Synthesis of 4-methyl-5-propoxymethoxazole from the propyl ester of  $\alpha$ -isocyanopropionic acid  
 AUTHOR(S): Mishchenko, V. V.; Itov, Z. I.; L'vova, S. D.;  
*Shostakovskaya, G. K.; Gunar, V. I.*  
 CORPORATE SOURCE: NPO "Vitaminy", Moscow, USSR  
 SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1988), 22(7),  
 856-60  
 DOCUMENT TYPE: CODEN: KHFZAN; ISSN: 0023-1134  
 LANGUAGE: Journal  
 Russian  
 OTHER SOURCE(S): CASREACT 110:114729  
 GI



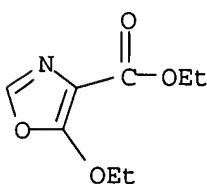
I

AB Thermal cyclization of Pr 2-isocyanopropionate 20 h at 135° gave 4-39% oxazole I depending on the solvent; higher yields were obtained with more polar solvents.  
 IT 19104-68-8P  
 RL: FORM (Formation, nonpreparative); PREP (Preparation)  
 (formation of, in thermal cyclization of Pr isocyanopropionate)  
 RN 19104-68-8 CAPLUS  
 CN Oxazole, 4-methyl-5-propoxy- (8CI, 9CI) (CA INDEX NAME)

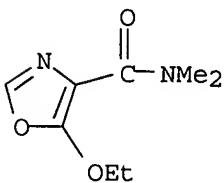


L8 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1975:458699 CAPLUS  
 DOCUMENT NUMBER: 83:58699

TITLE: *Syntheses with  $\alpha$ -metalated isocyanides. XXVIII.*  
*Oxazoles unsubstituted in position 2 from*  
 *$\alpha$ -metalated isocyanides and acylating reagents*  
 AUTHOR(S): Schroeder, Rolf; Schoellkopf, Ulrich; Blume, Ernst;  
 Hoppe, Inga  
 CORPORATE SOURCE: Org.-Chem. Inst., Univ. Goettingen, Goettingen, Fed.  
 Rep. Ger.  
 SOURCE: Justus Liebigs Annalen der Chemie (1975), (3), 533-46  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 OTHER SOURCE(S): CASREACT 83:58699  
 GI For diagram(s), see printed CA Issue.  
 AB Oxazoles I [R1 = Ph, CH2Ph, Me, Et, iso-Pr, OEt, tert-Bu, H,  
 1,2-epoxy-2-methylpropyl, p-tolyl; R = CO2Et, CONMe2, H, P(O)(OEt)2, Ph,  
 p-tolylthio, CH:CMe2] were prepared from  $\alpha$ -metalated isocyanides  
 $RC-HNC M^+$  ( $M = K, Li$ ) and acylating agents  $R_1COX$  ( $X = Cl, OEt, NMe_2$ ).  
 $\beta$ -Oxo isocyanides  $RCH(NC)COR_1$  are intermediates which cyclize either  
 in situ or during work-up.  $EtO_2CC-MeNC K^+$  and enolizable acyl chlorides  
 gave oxazolines II ( $R = H, Me$ ).  $EtO_2CC-HNC K^+$  and 0.5 equivalent  $EtO_2CCl$  gave  
 $EtO_2CCK(NC)CO_2Et$  which can be alkylated in situ by alkyl halides to give  
 $RC(NC)(CO_2Et)_2$  ( $R = Me, iso-Pr, CH_2CH:CH_2$ ), precursors of higher amino  
 acids.  
 IT 14423-15-5P 56157-42-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 14423-15-5 CAPLUS  
 CN 4-Oxazolecarboxylic acid, 5-ethoxy-, ethyl ester (8CI, 9CI) (CA INDEX  
 NAME)

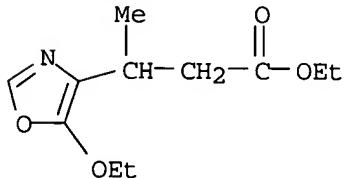


RN 56157-42-7 CAPLUS  
 CN 4-Oxazolecarboxamide, 5-ethoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)



L8 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1974:27048 CAPLUS  
 DOCUMENT NUMBER: 80:27048  
 TITLE: *Syntheses with  $\alpha$ -metalated isocyanides. XXIV.*  
*Syntheses of diethyl  $\alpha$ -isocyanoglutarates,*  
*glutamic acid derivatives, and pyrrolinecarboxylates*  
*from  $\alpha$ -isocyanoacetates or  $\alpha$ -*

AUTHOR(S): isocyanopropionates and acrylates  
 Schoellkopf, Ulrich; Hantke, Kurt  
 CORPORATE SOURCE: Org.-Chem. Inst., Univ. Goettingen, Goettingen, Fed.  
 Rep. Ger.  
 SOURCE: Justus Liebigs Annalen der Chemie (1973), 9, 1571-82  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 OTHER SOURCE(S): CASREACT 80:27048  
 GI For diagram(s), see printed CA Issue.  
 AB Michael addition of CNCHRCO<sub>2</sub>Et [R = H (I) or Me (II)] to R<sub>1</sub>CH:CR<sub>2</sub>CO<sub>2</sub>Et (R<sub>1</sub> = H, Me, Ph, CO<sub>2</sub>Et, or CH:CHMe; R<sub>2</sub> = H or Me) in EtOH at .apprx.50° in the presence of EtONa yielded 18-75% EtO<sub>2</sub>CCR(NC)CHR<sub>1</sub>CHR<sub>2</sub>CO<sub>2</sub>Et (III) and EtO<sub>2</sub>CC(NC)(CHR<sub>1</sub>CHR<sub>2</sub>CO<sub>2</sub>Et)<sub>2</sub>, resp. In dilute HCl, the NC group was converted into the NHCHO group. III (R = Me) were cyclized at .apprx.80° in the presence of equivalent amts. EtONa to give the pyrrolinecarboxylates IV and V, resp., which on hydrogenation gave the proline derivs. VI. Michael addition of I to PhCH:CHCOPh and of II to CH<sub>2</sub>:CHCOMe gave the pyrrolinecarboxylate VII and EtO<sub>2</sub>CCMe(NC)CH<sub>2</sub>CH<sub>2</sub>COMe, resp.  
 IT 50900-01-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 50900-01-1 CAPLUS  
 CN 4-Oxazolepropanoic acid, 5-ethoxy-β-methyl-, ethyl ester (9CI) (CA INDEX NAME)



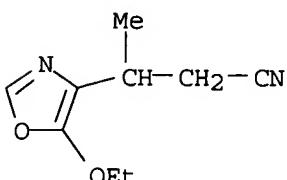
L8 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1974:27047 CAPLUS  
 DOCUMENT NUMBER: 80:27047  
 TITLE: Synthesis with α-metalated isocyanides. XXV.  
 Ethyl 4-cyano-2-isocyanoalkanoates, ethyl  
 4-cyano-2-(formylamino)alkanoates, and ethyl  
 4-cyano-5(4)-pyrroline-2-carboxylate from  
 α-metalated ethyl isocyanoalkanoates and  
 acrylonitriles  
 AUTHOR(S): Schoellkopf, Ulrich; Porsch, Paul H.  
 CORPORATE SOURCE: Org.-Chem. Inst., Univ. Goettingen, Goettingen, Fed.  
 Rep. Ger.  
 SOURCE: Chemische Berichte (1973), 106(10), 3382-90  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 GI For diagram(s), see printed CA Issue.  
 AB EtO<sub>2</sub>CCR(NC)CHR<sub>1</sub>CHR<sub>2</sub>CN (R, R<sub>2</sub> = H, Me; R<sub>1</sub> = H, Me, Ph) and EtO<sub>2</sub>CC(NC)(CHR<sub>1</sub>CHR<sub>2</sub>CN)<sub>2</sub> were prepared by reaction of R<sub>1</sub>CH:CR<sub>2</sub>CN (I) with EtO<sub>2</sub>CCHRN<sub>C</sub> (II) in EtOH at .apprx.30° in the presence of catalytic amts. EtONa. By treating with aqueous HCl, the **isocyano** group of the compds. obtained was converted into the formylamino group. Reaction of I with II in EtOH at .apprx.65° in the presence of equivalent amts.

EtONa yielded in the case of R2 = Me the pyrrolines III and in the case of R2 = H the pyrrolines IV.

IT 51068-91-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 51068-91-8 CAPLUS

CN 4-Oxazolepropanenitrile, 5-ethoxy- $\beta$ -methyl- (9CI) (CA INDEX NAME)

L8 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1969:68347 CAPLUS

DOCUMENT NUMBER: 70:68347

TITLE: 5-Alkoxy oxazole

INVENTOR(S): Maeda, Itsuki; Asai, Soichiro; Yoshida, Ryonosuke

PATENT ASSIGNEE(S): Ajinomoto Co., Inc.

SOURCE: Jpn. Tokkyo Koho, 4 pp.

CODEN: JAXXAD

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 43019953	B4	19680828	JP	19651104

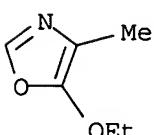
AB The title compds. are prepared by thermal cyclization of lower alkyl ester of  $\alpha$ -(isocyanato)alkylcarboxylic acid. Thus, 50 g. Et  $\alpha$ - isocyanato-propionate was kept at 180° for 3 hrs. in an autoclave. Fractional distillation of the reaction mixture gave 21.6 g. 5-ethoxy-4-methyloxazole b25 64-73°, (fraction A) and 19.3 g. unreacted fraction, b25 80-5°. Each fraction was subjected to gas chromatog. using a column of dinonyl phthalate on Teflon particles. Fraction A contained 95% product for a total yield of 78%.

IT 5006-20-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 5006-20-2 CAPLUS

CN Oxazole, 5-ethoxy-4-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



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L9 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2003-542425 CAPLUS  
 DOCUMENT NUMBER: 139:86982  
 TITLE: Process for the preparation of substituted oxazoles  
 INVENTOR(S): Rust, Harald; Burkart, Kirsten; Faust, Tillmann;  
 Henkelmann, Jochem; Kindler, Alois; Knoll, Christian;  
 Recker, Michael  
 PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany  
 SOURCE: U.S. Pat. Appl. Publ., 11 pp., Cont.-in-part of U.S.  
 Ser. No. 209,529.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003125567	A1	20030703	US 2003-348961	20030123
US 6900332	B2	20050531		
DE 10137480	A1	20030213	DE 2001-10137480	20010803
DE 10209446	A1	20030918	DE 2002-10209446	20020305
US 2003050479	A1	20030313	US 2002-209529	20020801
JP 2003176272	A2	20030624	JP 2002-227292	20020805
JP 2003267958	A2	20030925	JP 2002-355822	20021206
CN 1442412	A	20030917	CN 2002-156818	20021213
PRIORITY APPLN. INFO.:			DE 2001-10137480	A 20010803
			DE 2002-10209446	A 20020305
			US 2002-209529	A2 20020801

OTHER SOURCE(S): MARPAT 139:86982

AB The present invention relates to a process for preparing 5-alkoxy-substituted oxazoles, in particular for preparing 4-methyl-5-alkoxy-substituted oxazoles and also a process for preparing pyridoxine derivs. The process is carried out in a batchwise or semibatchwise reactor equipped with an emplaced reaction column and, simultaneously with the conversion, removing the 5-alkoxy-substituted oxazoles from the reaction mixture by rectification provided that the parameters of the rectification are set in such a way that the  $\alpha$ - isocyanoalkanoate esters are converted to the 5-alkoxy-substituted oxazoles in the reactor and/or on the internals of the emplaced reaction column and the 5-alkoxy-substituted oxazoles resulting from the conversion are removed via the emplaced reaction column.

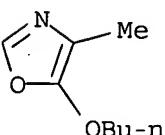
IT 24201-52-3P, 5-Butoxy-4-methyloxazole

RL: IMF (Industrial manufacture); PREP (Preparation)

(batchwise or semibatchwise process for preparation of substituted oxazoles)

RN 24201-52-3 CAPLUS

CN Oxazole, 5-butoxy-4-methyl- (8CI, 9CI) (CA INDEX NAME)

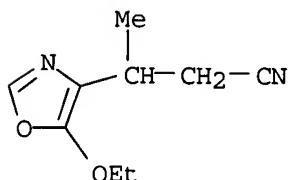


ACCESSION NUMBER: 1974:27047 CAPLUS  
 DOCUMENT NUMBER: 80:27047  
 TITLE: Synthesis with  $\alpha$ -metalated isocyanides. XXV.  
 Ethyl 4-cyano-2-isocyanoalkanoates, ethyl  
 4-cyano-2-(formylamino)alkanoates, and ethyl  
 4-cyano-5(4)-pyrroline-2-carboxylate from  
 $\alpha$ -metalated ethyl isocyanoalkanoates  
 and acrylonitriles

AUTHOR(S): Schoellkopf, Ulrich; Porsch, Paul H.  
 CORPORATE SOURCE: Org.-Chem. Inst., Univ. Goettingen, Goettingen, Fed.  
 Rep. Ger.  
 SOURCE: Chemische Berichte (1973), 106(10), 3382-90  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 GI For diagram(s), see printed CA Issue.  
 AB EtO<sub>2</sub>CCR(NC)CHR<sub>1</sub>CHR<sub>2</sub>CN (R, R<sub>2</sub> = H, Me; R<sub>1</sub> = H, Me, Ph) and  
 EtO<sub>2</sub>CC(NC)(CHR<sub>1</sub>CHR<sub>2</sub>CN)<sub>2</sub> were prepared by reaction of R<sub>1</sub>CH:CR<sub>2</sub>CN (I) with  
 EtO<sub>2</sub>CCHRN<sub>C</sub> (II) in EtOH at .apprx.30° in the presence of catalytic  
 amts. EtONa. By treating with aqueous HCl, the isocyano group of the compds.  
 obtained was converted into the formylamino group. Reaction of I with II  
 in EtOH at .apprx.65° in the presence of equivalent amts. EtONa yielded  
 in the case of R<sub>2</sub> = Me the pyrrolines III and in the case of R<sub>2</sub> = H the  
 pyrrolines IV.

IT 51068-91-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 51068-91-8 CAPLUS  
 CN 4-Oxazolepropanenitrile, 5-ethoxy- $\beta$ -methyl- (9CI) (CA INDEX NAME)



L9 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1971:448961 CAPLUS  
 DOCUMENT NUMBER: 75:48961  
 TITLE: Synthetic intermediate of pyridoxine. II. Thermal  
 cyclization of ethyl  $\alpha$ -isocyanopropionate to  
 5-ethoxy-4-methyloxazole

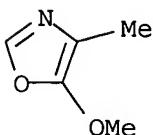
AUTHOR(S): Maeda, Itsutoshi; Togo, Kazushi; Yoshida, Ryonosuke  
 CORPORATE SOURCE: Cent. Res. Lab., Ajinomoto Co., Inc., Kawasaki, Japan  
 SOURCE: Bulletin of the Chemical Society of Japan (1971),  
 44(5), 1407-10  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI For diagram(s), see printed CA Issue.  
 AB The thermal cyclization of ethyl  $\alpha$ -isocyanopropionate (I) gave  
 5-ethoxy-4-methyloxazole (II) as an intermediate for the synthesis of  
 pyridoxine. The similar reaction of several alkyl esters of  
 $\alpha$ -isocyanocarboxylic acid to the corresponding 5-alkoxy-4-  
 substituted oxazole was also carried out. The products of the thermal

cyclization of I were investigated. When the cyclization was carried out 5 hr at 180°, the maximum yield of the main product, II, was 20%; unreacted I (30%), Et α-cyanopropionate (20%), and dimer of I (5%) were also obtained. The α-H of Et α-isocyanosuccinate (III) can be more easily removed than that of I, so III may be expected to be more readily converted to 5-ethoxy-4-ethoxycarbonylmethyloxazole (IV), which is also an intermediate of pyridoxine. The yield of IV from III was <30% because of the side reaction.

IT 1622-76-0P 5006-20-2P 5214-69-7P  
 15031-12-6P 24201-52-3P 33115-82-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

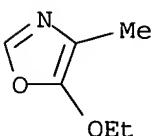
RN 1622-76-0 CAPLUS

CN Oxazole, 5-methoxy-4-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



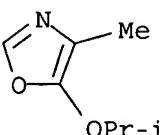
RN 5006-20-2 CAPLUS

CN Oxazole, 5-ethoxy-4-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



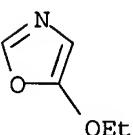
RN 5214-69-7 CAPLUS

CN Oxazole, 4-methyl-5-(1-methylethoxy)- (9CI) (CA INDEX NAME)



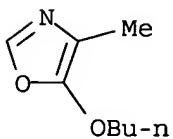
RN 15031-12-6 CAPLUS

CN Oxazole, 5-ethoxy- (8CI, 9CI) (CA INDEX NAME)

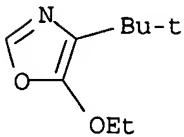


RN 24201-52-3 CAPLUS

CN Oxazole, 5-butoxy-4-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 33115-82-1 CAPLUS  
 CN Oxazole, 5-ethoxy-4-isobutyl- (8CI) (CA INDEX NAME)

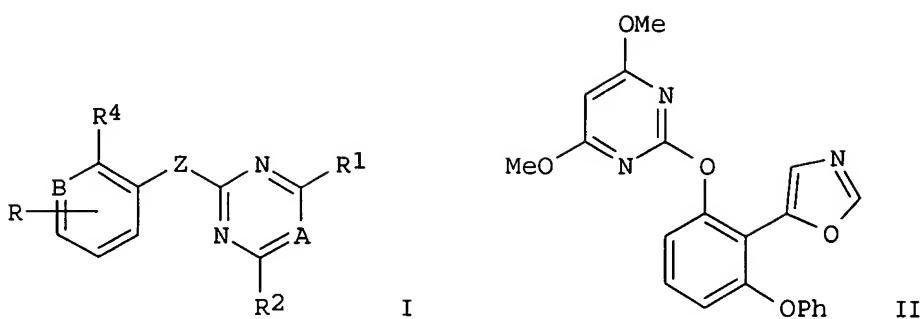


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L13 ANSWER 1 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2001:560055 CAPLUS  
 DOCUMENT NUMBER: 135:137518  
 TITLE: Preparation of pyrimidinylphenyloxazole derivatives as herbicides  
 INVENTOR(S): Ueda, Akiyoshi; Miyazawa, Yasuyuki; Hara, Yoshihiko; Koguchi, Masami; Takahashi, Akihiro; Kawana, Takashi  
 PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan  
 SOURCE: U.S., 41 pp., Cont.-in-part of U.S. 5,962,685.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6268310	B1	20010731	US 1999-248372	19990210 <--
US 5962685	A	19991005	US 1997-750932	19970128 <--
PRIORITY APPLN. INFO.:			US 1997-750932	A2 19970128
			JP 1994-200196	A 19940802
			JP 1994-200197	A 19940802
			WO 1995-JP1523	W 19950801

OTHER SOURCE(S): MARPAT 135:137518  
 GI



**AB** Title compds. [I; A = N or CR<sub>3</sub>; B = N or an (un)substituted C (sic); R = H or 1-4 of (halo)alkyl, alkenyl, alkynyl, etc.; ; R<sub>1</sub>,R<sub>2</sub> = H, C<sub>1</sub>-6 (halo)alkyl, C<sub>1</sub>-6 (halo)alkoxy, etc.; R<sub>3</sub> = H, C<sub>1</sub>-6 alkyl, halo, NO<sub>2</sub>, CHO, acyl; R<sub>4</sub> = (un)substituted oxazolyl; Z = O or SOO-2] were prepared Thus, title compound II (preparation given) at 2.5 g/are gave 100% control of barnyard

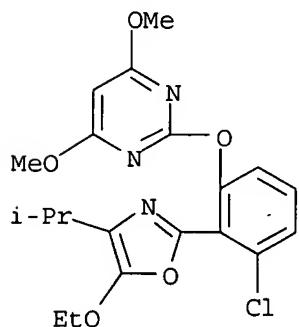
grass, Cyperus diffiformis, and Scirpus juncoides.

**IT** 177708-92-8P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of pyrimidinylphenyloxazole derivs. as herbicides)

**RN** 177708-92-8 CAPLUS

**CN** Pyrimidine, 2-[3-chloro-2-[5-ethoxy-4-(1-methylethyl)-2-oxazolyl]phenoxy]-4,6-dimethoxy- (9CI) (CA INDEX NAME)



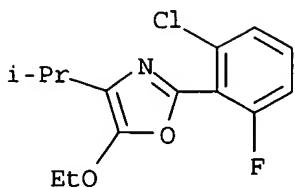
**IT** 177710-95-1P 177710-96-2P 177710-97-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

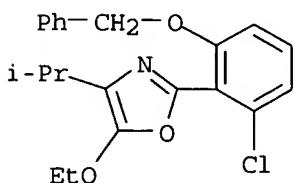
(preparation of pyrimidinylphenyloxazole derivs. as herbicides)

**RN** 177710-95-1 CAPLUS

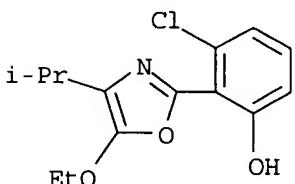
**CN** Oxazole, 2-(2-chloro-6-fluorophenyl)-5-ethoxy-4-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 177710-96-2 CAPLUS  
 CN Oxazole, 2-[2-chloro-6-(phenylmethoxy)phenyl]-5-ethoxy-4-(1-methylethyl)-  
 (9CI) (CA INDEX NAME)



RN 177710-97-3 CAPLUS  
 CN Phenol, 3-chloro-2-[5-ethoxy-4-(1-methylethyl)-2-oxazolyl]- (9CI) (CA  
 INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1999:529133 CAPLUS  
 DOCUMENT NUMBER: 131:157711  
 TITLE: Preparation of pyridinecarboxylates and analogs as  
 cholestryl ester transfer protein inhibitors  
 INVENTOR(S): Lee, Len F.; Glenn, Kevin C.; Connolly, Daniel T.;  
 Corley, David G.; Flynn, Daniel L.; Hamme, Ashton;  
 Hegde, Shridhar G.; Melton, Michele A.; Schilling,  
 Roger J.; Sikorski, James A.; Wall, Nancy N.;  
 Zablocki, Jeffrey A.  
 PATENT ASSIGNEE(S): G.D. Searle and Co., USA  
 SOURCE: PCT Int. Appl., 327 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

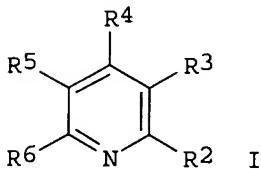
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 9941237	A1	19990819	WO 1999-US1871	19990211 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9932854	A1	19990830	AU 1999-32854	19990211 <--
US 6605624	B1	20030812	US 2000-600870	20001211 <--
US 2004038939	A1	20040226	US 2003-403903	20030331 <--
US 6794396	B2	20040921		
US 2004220231	A1	20041104	US 2004-852975	20040525 <--
PRIORITY APPLN. INFO.:			US 1998-74586P	P 19980213
			WO 1999-US1871	W 19990211
			US 2000-600870	A3 20001211
			US 2003-403903	A3 20030331

OTHER SOURCE(S) : MARPAT 131:157711

GI



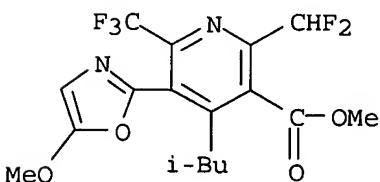
AB Title compds. [I; R2,R6 = H, OH, (fluoro)alkyl, alkoxy, etc.; R3 = OH, CHO, alkoxy carbonyl, (hetero)aryl carbonyl, etc.; R5 = H, halo, alkyl, alkoxy, etc.; R5 = H, halo, alkyl, alkoxy (carbonyl), etc.] were prepared. Thus, CF<sub>3</sub>C(NH<sub>2</sub>):C(CO<sub>2</sub>Me)COMe was refluxed with Ac<sub>2</sub>O/HC(OMe)<sub>3</sub> and the product converted in 2 steps to I (R2 = CF<sub>3</sub>, R3 = CO<sub>2</sub>Me, R4 = OCHMe<sub>2</sub>, R5 = R6 = H). Data for biol. activity of I were given.

IT 117718-35-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of pyridinecarboxylates and analogs as cholesteryl ester transfer protein inhibitors)

RN 117718-35-1 CAPLUS

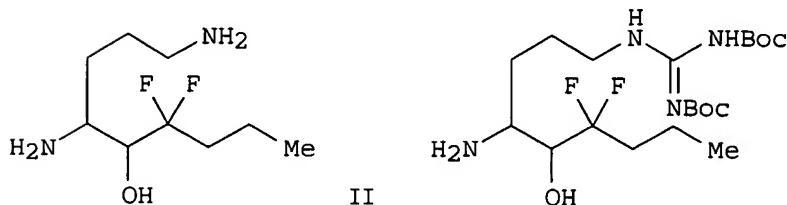
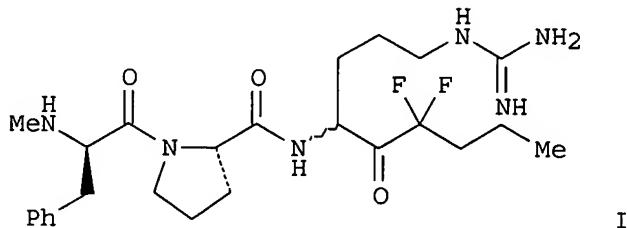
CN 3-Pyridinecarboxylic acid, 2-(difluoromethyl)-5-(5-methoxy-2-oxazolyl)-4-(2-methylpropyl)-6-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT.

L13 ANSWER 3 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1998:226851 CAPLUS  
DOCUMENT NUMBER: 128:283091  
TITLE: Process for the preparation of N-methyl-D-phenylalanyl-N-[1-[3-[(aminoiminomethyl)amino]propyl]-3,3-difluoro-2-oxohexyl]-L-prolinamide by direct guanylation of Dakin-West intermediates  
INVENTOR(S): Rudisill, Duane E.  
PATENT ASSIGNEE(S): Hoechst Marion Roussel, Inc., USA  
SOURCE: U.S., 12 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5739354	A	19980414	US 1997-786997	19970123 <--
PRIORITY APPLN. INFO.:			US 1997-786997	19970123
OTHER SOURCE(S):	CASREACT	128:283091		
GI				



AB The present invention relates to a novel process for preparing the title compound (MDL 75,579DA) (I) or a pharmaceutically acceptable salt thereof and to a key intermediate by directly guanylating Dakin-West intermediates. Thus, direct guanylation of 9,6-diamino-5-hydroxy-4,4-difluoronoronane (II; prepared in 6 steps from Et 2,2-difluoro-4-pentenoate and N8-benzyloxycarbonyl-L-ornithine) with (bis-Boc-amidino)pyrazole (Boc = Me<sub>3</sub>CO<sub>2</sub>C) gave protected guanidine derivative III in 83% yield. III was converted into I via peptide coupling with N-Boc-N-methyl-D-phenylalanyl-L-proline, Swern oxidation, and deprotection.

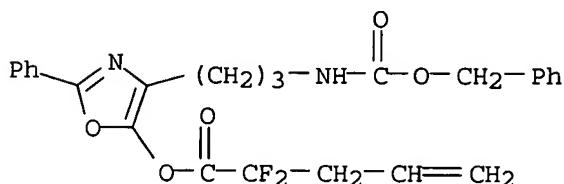
IT 170887-02-2P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic

preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (process for preparation of thrombin inhibitor MDL 75,579DA via direct  
 guanylation of Dakin-West intermediates)

RN 170887-02-2 CAPLUS

CN 4-Pentenoic acid, 2,2-difluoro-, 2-phenyl-4-[3-  
 [(phenylmethoxy)carbonyl]amino]propyl]-5-oxazolyl ester (9CI) (CA INDEX  
 NAME)



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:394187 CAPLUS

DOCUMENT NUMBER: 127:5094

TITLE: N-Heterocyclylcarbonylbenzene- and -thiophenesulfonamides as herbicides

INVENTOR(S): Mueller, Klaus-Helmut; Drewes, Mark Wilhelm;  
 Findeisen, Kurt; Gesing, Ernst R. F.; Jansen, Johannes  
 R.; Kirsten, Rolf; Kluth, Joachim; Philipp, Ulrich;  
 Riebel, Hans-Joachim; Dollinger, Markus; Santel,  
 Hans-Joachim

PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Ger. Offen., 51 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

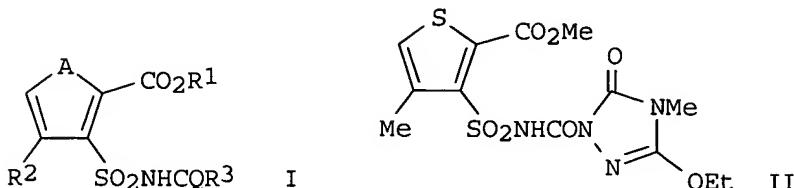
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19540737	A1	19970507	DE 1995-19540737	19951102 <--
CA 2236208	AA	19970509	CA 1996-2236208	19961021 <--
CA 2236208	C	20050503		
WO 9716449	A1	19970509	WO 1996-EP4559	19961021 <--
W: AU, BB, BG, BR, BY, CA, CN, CZ, HU, JP, KR, KZ, LK, MX, NO, NZ, PL, RO, RU, SK, TR, UA, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9674909	A1	19970522	AU 1996-74909	19961021 <--
EP 859774	A1	19980826	EP 1996-937202	19961021 <--
EP 859774	B1	20020403		
R: DE, FR, GB, IT				
CN 1207099	A	19990203	CN 1996-199468	19961021 <--
CN 1105717	B	20030416		
BR 9611129	A	19990330	BR 1996-11129	19961021 <--
JP 11515018	T2	19991221	JP 1996-517028	19961021 <--
PL 186726	B1	20040227	PL 1996-327978	19961021
US 6180567	B1	20010130	US 1998-66385	19980807 <--

US 6441195	B1	20020827	US 2000-710079	20001109 <--
CN 1439631	A	20030903	CN 2002-104506	20020207
US 2003162979	A1	20030828	US 2002-137088	20020501 <--
PRIORITY APPLN. INFO.:				
			DE 1995-19540737	A 19951102
			WO 1996-EP4559	W 19961021
			US 1998-66385	A3 19980807
			US 2000-710079	A3 20001109

OTHER SOURCE(S) : MARPAT 127:5094  
GI

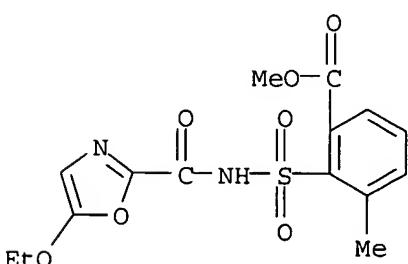


AB Title compds. I [A = O, S, (un)substituted NH, CH:N, N:CH, CH:CH; Q = O, . . . S; R1 = alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl, heterocyclyl, heterocyclylalkyl; R2 = CN, NO<sub>2</sub>, halogen, (un)substituted alkyl, alkoxy, alkoxy carbonyl, alkylthio, alkylsulfinyl, alkylsulfonyl, alkenyl, alkynyl, alkenyloxy, alkynyoxy; R3 = (un)substituted 5-membered heterocycle] and their salts were prepared. Thus, the triazole derivative II was obtained from the thiophenesulfonamide and the triazolecarboxylate. II has herbicidal activity while being well tolerated by maize and soybeans.

IT 190374-20-0P 190374-21-1P  
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of N-heterocyclylcarbonylbenzene- and -thiophenesulfonamides as herbicides)

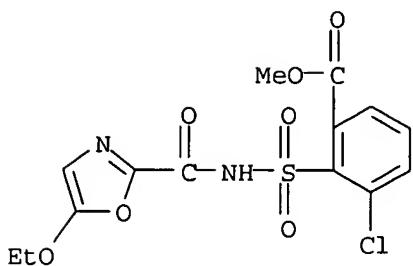
RN 190374-20-0 CAPLUS

CN Benzoic acid, 2-[[[(5-ethoxy-2-oxazolyl)carbonyl]amino]sulfonyl]-3-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 190374-21-1 CAPLUS

CN Benzoic acid, 3-chloro-2-[[[(5-ethoxy-2-oxazolyl)carbonyl]amino]sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 5 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:369768 CAPLUS

DOCUMENT NUMBER: 126:343564

TITLE: Process for the preparation of nitriles by the  
dehydration of amides in the presence of sulfur  
trioxide-amine dehydration agents

INVENTOR(S): Bonrath, Werner; Pauling, Horst

PATENT ASSIGNEE(S): F. Hoffmann-La Roche Ag, Switz.

SOURCE: Eur. Pat. Appl., 5 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 775691	A1	19970528	EP 1996-118232	19961114 <--
EP 775691	B1	20000126		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL				
US 5817827	A	19981006	US 1996-734987	19961022 <--
JP 09169714	A2	19970630	JP 1996-283700	19961025 <--
CN 1156721	A	19970813	CN 1996-114461	19961113 <--
CN 1071311	B	20010919		
AT 189209	E	20000215	AT 1996-118232	19961114 <--
ES 2143126	T3	20000501	ES 1996-118232	19961114 <--
			CH 1995-3290	A 19951121

PRIORITY APPLN. INFO.:

OTHER SOURCE(S): CASREACT 126:343564

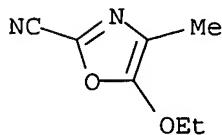
AB Nitriles (e.g., 5-cyano-4-methyloxazole) are prepared in high yield and  
selectivity by the dehydration of amides (e.g., 5-carbamoyl-4-  
methyloxazole) in the presence of SO<sub>3</sub> and a tertiary amine (e.g., Et<sub>3</sub>N).

IT 189807-90-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(process for the preparation of nitriles by the dehydration of amides in the  
presence of sulfur trioxide-amine dehydration agents)

RN 189807-90-7 CAPLUS

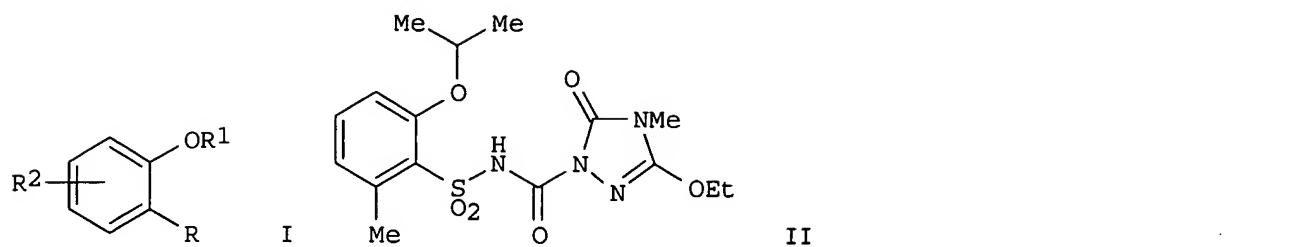
CN 2-Oxazolecarbonitrile, 5-ethoxy-4-methyl- (9CI) (CA INDEX NAME)



L13 ANSWER 6 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1997:191906 CAPLUS  
 DOCUMENT NUMBER: 126:186088  
 TITLE: Preparation of 2-[(phenylsulfonyl)aminocarbonyl]-1,2,4-triazol-3-ones and analogs as herbicides  
 INVENTOR(S): Mueller, Klaus-Helmut; Kirsten, Rolf; Gesing, Ernst R. F.; Kluth, Joachim; Drewes, Mark Wilhelm; Findeisen, Kurt; Jansen, Johannes R.; Koenig, Klaus; Riebel, Hans-Jochem; Schallner, Otto; Dollinger, Markus; Santel, Hans-Joachim  
 PATENT ASSIGNEE(S): Bayer A.-G., Germany  
 SOURCE: Ger. Offen., 115 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19525162	A1	19970116	DE 1995-19525162	19950711 <--
CA 2226669	AA	19970130	CA 1996-2226669	19960628 <--
WO 9703056	A1	19970130	WO 1996-EP2826	19960628 <--
W: AU, BB, BG, BR, BY, CA, CN, CZ, HU, JP, KR, KZ, LK, MX, NO, NZ, PL, RO, RU, SK, TR, UA, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9665146	A1	19970210	AU 1996-65146	19960628 <--
AU 703153	B2	19990318		
EP 842157	A1	19980520	EP 1996-924805	19960628 <--
EP 842157	B1	20030827		
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
CN 1198159	A	19981104	CN 1996-196753	19960628 <--
CN 1086696	B	20020626		
BR 9609902	A	19990629	BR 1996-9902	19960628 <--
JP 11508595	T2	19990727	JP 1996-505456	19960628 <--
EP 1344771	A1	20030917	EP 2003-11479	19960628
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
ES 2202457	T3	20040401	ES 1996-924805	19960628
ZA 9605841	A	19970131	ZA 1996-5841	19960710 <--
US 6251831	B1	20010626	US 1998-223246	19981230 <--
HK 1016167	A1	20030228	HK 1999-101110	19990317
CN 1316418	A	20011010	CN 2001-101527	20010117
US 6525211	B1	20030225	US 2001-838812	20010420 <--
PRIORITY APPLN. INFO.:			DE 1995-19525162	A 19950711
			EP 1996-924805	A3 19960628
			WO 1996-EP2826	W 19960628
			US 1998-6686	B1 19980108
			US 1998-223246	A3 19981230

OTHER SOURCE(S): MARPAT 126:186088  
 GI



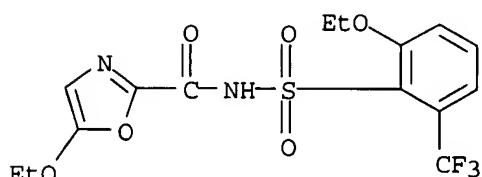
AB Title compds. [I; R = ZSO<sub>2</sub>NHC(:X)R<sub>3</sub>; R<sub>1</sub> = H, CHO, (un)substituted alk(en)yl, acyl, etc.; R<sub>2</sub> = halo, cyano, alkyl, alkoxy, etc.; R<sub>3</sub> = heterocyclyl; X = O or S; Z = bond, O, S, (alkyl)imino, etc.] were prepared as herbicides (no data). Thus, Ph 5-ethoxy-4-methyl-2,4-dihydro-3H-1,2,4-triazol-3-one-2-carboxylate was amidated by 2,6-Me(Me<sub>2</sub>HCO)C<sub>6</sub>H<sub>3</sub>SO<sub>2</sub>NH<sub>2</sub> to give title compound II.

IT 187469-45-0P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 2-[(phenylsulfonyl)aminocarbonyl]-1,2,4-triazol-3-ones and analogs as herbicides)

RN 187469-45-0 CAPLUS

CN 2-Oxazolecarboxamide, 5-ethoxy-N-[2-ethoxy-6-(trifluoromethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



L13 ANSWER 7 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:363369 CAPLUS

DOCUMENT NUMBER: 125:33668

TITLE: Preparation of pyrimidinylphenyloxazole derivatives as herbicides

INVENTOR(S) : Ueda, Akiyoshi; Miyazawa, Yasuyuki; Hara, Yoshihiko;  
Koguchi, Masami; Takahashi, Akihiro; Kawana, Takashi

PATENT ASSIGNEE(S) : Nippon Soda Co., Ltd., Japan

SOURCE: PCT Int. Appl., 111 pp.

CODEN: PIXXD2

DOCUMENT TYPE: **Patent**

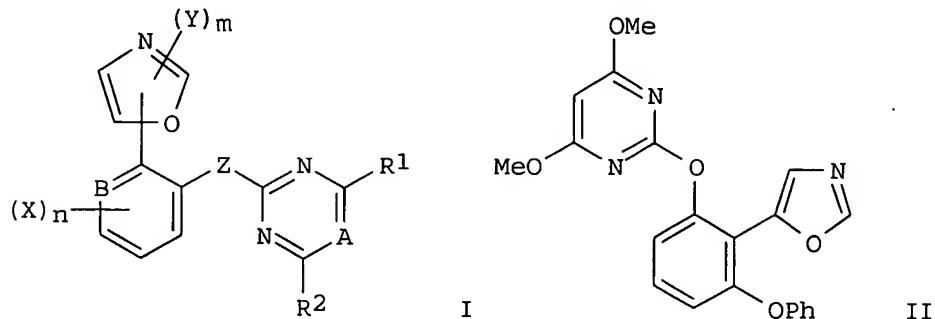
**LANGUAGE:**

FAMILY ACC. NUM. CO

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9604278	A1	19960215	WO 1995-JP1523	19950801 <--
W: AU, BR, CA, CN, HU, JP, KR, RU, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9530871	A1	19960304	AU 1995-30871	19950801 <--

EP 776894	A1	19970604	EP 1995-926531	19950801 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
US 5962685	A	19991005	US 1997-750932	19970128 <--
US 6107251	A	20000822	US 1999-249650	19990212 <--
PRIORITY APPLN. INFO. :			JP 1994-200196	A 19940802
			JP 1994-200197	A 19940802
			WO 1995-JP1523	W 19950801

OTHER SOURCE(S) : MARPAT 125:33668  
GI

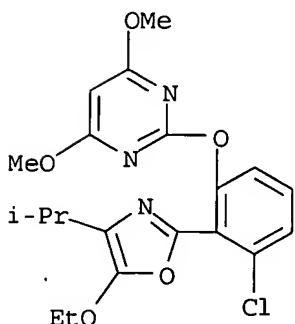


AB The title compds. I [A represents a nitrogen atom or an R<sub>3</sub>-substituted carbon atom; B represents a nitrogen atom, or an unsubstituted or X-substituted carbon atom; Z represents oxygen, S, sulfinyl or sulfonyl; R<sub>1</sub> and R<sub>2</sub> represent each independently hydrogen, C<sub>1</sub>-C<sub>6</sub> alkyl, C<sub>1</sub>-C<sub>6</sub> alkoxy, C<sub>1</sub>-C<sub>6</sub> haloalkoxy, C<sub>1</sub>-C<sub>6</sub> haloalkyl, etc.; R<sub>3</sub> represents hydrogen, C<sub>1</sub>-C<sub>6</sub> alkyl, halogeno, nitro, formyl or acyl; X represents hydrogen, C<sub>1</sub>-C<sub>6</sub> alkyl, C<sub>3</sub>-C<sub>7</sub> cycloalkyl, C<sub>2</sub>-C<sub>6</sub> alkenyl, C<sub>3</sub>-C<sub>6</sub> alkynyl, C<sub>1</sub>-C<sub>6</sub> haloalkyl, etc.; Y represents hydrogen, C<sub>1</sub>-C<sub>6</sub> alkyl, C<sub>3</sub>-C<sub>7</sub> cycloalkyl, C<sub>2</sub>-C<sub>6</sub> alkenyl, C<sub>3</sub>-C<sub>6</sub> alkynyl, C<sub>1</sub>-C<sub>6</sub> haloalkyl, etc.; m represents an integer of 1 or 2; and n represents an integer of 1 to 4] are prepared. The title compound II (preparation given) (at 2.5 g/are) gave 100% control of barnyard grass, Cyperus difformis, and Scirpus juncooides.

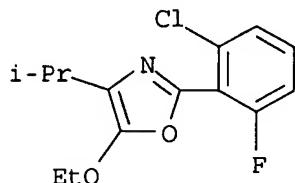
IT 177708-92-8P  
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of pyrimidinylphenyloxazole derivs. as herbicides)

RN 177708-92-8 CAPLUS

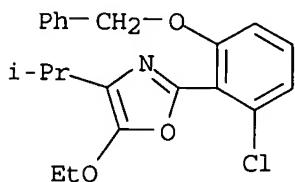
CN Pyrimidine, 2-[3-chloro-2-[5-ethoxy-4-(1-methylethyl)-2-oxazolyl]phenoxy]-4,6-dimethoxy- (9CI) (CA INDEX NAME)



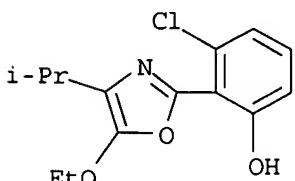
IT 177710-95-1P 177710-96-2P 177710-97-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of pyrimidinylphenyloxazole derivs. as herbicides)  
 RN 177710-95-1 CAPLUS  
 CN Oxazole, 2-(2-chloro-6-fluorophenyl)-5-ethoxy-4-(1-methylethyl)- (9CI)  
 (CA INDEX NAME)



RN 177710-96-2 CAPLUS  
 CN Oxazole, 2-[2-chloro-6-(phenylmethoxy)phenyl]-5-ethoxy-4-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 177710-97-3 CAPLUS  
 CN Phenol, 3-chloro-2-[5-ethoxy-4-(1-methylethyl)-2-oxazolyl]- (9CI) (CA INDEX NAME)



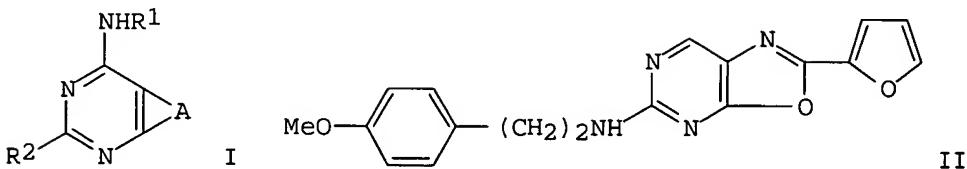
L13 ANSWER 8 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1993:560314 CAPLUS  
 DOCUMENT NUMBER: 119:160314  
 TITLE: Preparation of furyl-substituted purines,  
 oxazolopyrimidines and pteridines as adenosine  
 antagonists  
 INVENTOR(S): Block, Michael Howard; Harrison, Alison; Hargreaves,  
 Rodney Brian  
 PATENT ASSIGNEE(S): Imperial Chemical Industries PLC, UK  
 SOURCE: Eur. Pat. Appl., 23 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent

LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 544445	A2	19930602	EP 1992-310544	19921119 <--
EP 544445	A3	19931103		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CA 2082333	AA	19930526	CA 1992-2082333	19921106 <--
US 5300509	A	19940405	US 1992-979019	19921120 <--
JP 06157540	A2	19940603	JP 1992-315388	19921125 <--
US 5500428	A	19960319	US 1994-181202	19940113 <--
PRIORITY APPLN. INFO.:			GB 1991-25001	A 19911125
			US 1992-979019	A3 19921120

OTHER SOURCE(S): MARPAT 119:160314

GI



AB Title compds. I (R1 = H, C1-6 alkyl, C1-4 alkanoyl; R2 = H, NC, XR3 wherein X = bond, O, S, SO, SO2 imino, R3 = C3-12 cycloalkyl, (substituted) C1-6 alkyl, (substituted) Ph, R4(CO)nXa(CO)m wherein R4 = C1-6 alkyl, C3-6 cycloalkyl, (substituted) Ph, etc., Xa = X, m, n = 0, 1; A = N:CQO, N:CQNR8, N:CQCH:N, N:CHCQ:N wherein Q = 2-furyl, R8 = H, C1-4 alkyl with a proviso) or a salt thereof, are prepared 4,6-Dihydroxy-5-(2-furanylcarbonyl)amino-2-[(4-methoxyphenyl)ethyl]aminopyrimidine (preparation given) and POCl3 were heated at 90° for 3 h to give 7-chloro-2-(2-furyl)-5-[2-(4-methoxyphenyl)ethyl]aminoxazol[5,4-d]pyrimidine which with NH4Cl were added to a saturated solution of NH3/EtOH to give title compound II which in A2 adenosine receptor affinity test showed a pIC50 >7 vs. 1,3-dimethylxanthine showing pIC50 of 5. Capsule and tablet formulations comprising I are given.

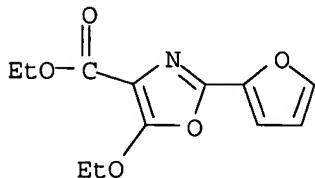
IT 149849-02-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of adenosine antagonists)

RN 149849-02-5 CAPLUS

CN 4-Oxazolecarboxylic acid, 5-ethoxy-2-(2-furanyl)-, ethyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 9 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1992:571465 CAPLUS  
 DOCUMENT NUMBER: 117:171465  
 TITLE: Chemiluminescent pyridopyridazines and their use  
 INVENTOR(S): Masuya, Hirotomo; Kondo, Koichi; Aramaki, Yoshio;  
 Ichimori, Yuzo  
 PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan  
 SOURCE: Eur. Pat. Appl., 48 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 491477	A1	19920624	EP 1991-310875	19911126 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
CA 2056142	AA	19920528	CA 1991-2056142	19911125 <--
JP 05078356	A2	19930330	JP 1991-312347	19911127 <--
JP 3167762	B2	20010521		
US 5420275	A	19950530	US 1993-144505	19931102 <--
PRIORITY APPLN. INFO.:			JP 1990-327777	A 19901127
			US 1991-799083	B1 19911127

OTHER SOURCE(S): MARPAT 117:171465

GI For diagram(s), see printed CA Issue.

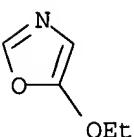
AB Title compds. I [R1 = (un)substituted hydroxycarbyl, heterocyclyl; R2 = OH, SH, (un)substituted NH2; R1R2 = azaalkylene; R3 = H, (un)substituted (OH, SH, NH2, CO2H, CONH2), halo, heterocyclyl, NO2, CN, N3, sulfo, sulfonyl; X = O, S] were prepared. Thus, I (R1 = Ph, R2 = NH2, R3 = Cl, X = O, II) was prepared from EtO(H2N)C:CHCO2Et and PhCOCH2CO2Et via cyclocondensation of 3-amino-6-chloro-4,5-diethoxycarbonyl-2-phenylpyridine with NH2NH2·H2O at 100°. In the presence of 1 pg horseradish peroxidase 0.2 mM II provided 0.678 kilocount chemiluminescence cf. luminol 0.032 kilocount.

IT 15031-12-6P, 5-Ethoxyoxazole

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction of, with di-Me fumarate)

RN 15031-12-6 CAPLUS

CN Oxazole, 5-ethoxy- (8CI, 9CI) (CA INDEX NAME)



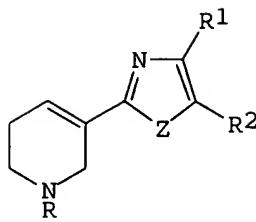
L13 ANSWER 10 OF 30 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:81822 CAPLUS  
 DOCUMENT NUMBER: 114:81822  
 TITLE: Preparation of 1,2,5,6-tetrahydropyrimidylloxazoles or -thiazoles as stimulants of cognitive function  
 INVENTOR(S): Sauerberg, Per; Olesen, Preben H.; Mitch, Charles H.  
 PATENT ASSIGNEE(S): Aktieselskabet Ferrosan, Den.  
 SOURCE: Eur. Pat. Appl., 11 pp.

CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 384285	A2	19900829	EP 1990-102889	19900214 <--
EP 384285	A3	19910424		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL				
DK 8900825	A	19900823	DK 1989-825	19890222 <--
US 5043345	A	19910827	US 1989-401370	19890831 <--
IL 93352	A1	19940826	IL 1990-93352	19900212 <--
ES 2072323	T3	19950716	ES 1990-102913	19900214 <--
AU 9049996	A1	19900830	AU 1990-49996	19900220 <--
AU 9049997	A1	19900830	AU 1990-49997	19900220 <--
AU 629302	B2	19921001		
US 5041455	A	19910820	US 1990-482272	19900220 <--
CA 2010578	AA	19900822	CA 1990-2010578	19900221 <--
CA 2010578	C	20000523		
CA 2010579	AA	19900822	CA 1990-2010579	19900221 <--
NO 9000830	A	19900823	NO 1990-830	19900221 <--
NO 179639	B	19960812		
NO 179639	C	19961120		
NO 9000831	A	19900823	NO 1990-831	19900221 <--
HU 58326	A2	19920228	HU 1990-884	19900221 <--
RU 2042676	C1	19950827	RU 1990-4743296	19900221 <--
KR 163763	B1	19981201	KR 1990-2108	19900221 <--
CN 1045104	A	19900905	CN 1990-100873	19900222 <--
CN 1028105	B	19950405		
JP 02255679	A2	19901016	JP 1990-39899	19900222 <--
JP 2921578	B2	19990719		
JP 02255680	A2	19901016	JP 1990-39900	19900222 <--
ZA 9001349	A	19901128	ZA 1990-1349	19900222 <--
ZA 9001350	A	19901128	ZA 1990-1350	19900222 <--
FI 95704	B	19951130	FI 1990-886	19900222 <--
FI 95704	C	19960311		
US 5264444	A	19931123	US 1991-744725	19910814 <--
US 5284859	A	19940208	US 1991-745568	19910815 <--
US 5328925	A	19940712	US 1991-746104	19910815 <--
US 5260311	A	19931109	US 1991-746378	19910816 <--
US 5559138	A	19960924	US 1995-472356	19950607 <--
US 5712297	A	19980127	US 1996-717647	19960923 <--
PRIORITY APPLN. INFO.:			DK 1989-825	A 19890222
			DK 1989-2315	A 19890512
			US 1989-401370	A2 19890831
			US 1990-482272	A1 19900220
			US 1991-745568	A3 19910815
			US 1993-144951	B1 19931029
			US 1995-472356	A3 19950607

OTHER SOURCE(S): MARPAT 114:81822  
 GI



**AB** The title compds. I ( $R = H$ , C1-3 alkyl, C3-4 cycloalkyl, C2-4 alkenyl, C2-4 alkynyl;  $R1, R2 = C1-10$  alkyl, C2-10 alkenyl, C2-10 alkynyl, C1-10 alkoxy, C3-10 cycloalkyl, etc.;  $Z = O, S$ ) or their salts, useful as stimulants of cognitive function, especially in treatment of Alzheimer's disease, were prepared  $(COCl)_2$  was added to arecaidine-HCl in  $CH_2Cl_2$ , followed by DMF, the reaction mixture refluxed for 3 h, cooled, to this solution was added (2S,3S)-EtCHMeCH(NH<sub>2</sub>)CO<sub>2</sub>Pr·HCl (preparation given), the resulting mixture refluxed for 48 h to give (S)-I ( $R = Me$ ,  $R1 = EtCHMe$ ,  $R2 = PrO$ ,  $Z = O$ ) as its maleate salt. (S)-I.maleate ( $R = Me$ ,  $R1 = EtCHMe$ ,  $R2 = MeO$ ;  $Z = O$ ) at 3.7 ng/mL had an IC<sub>50</sub> for in vitro binding of 3H-oxotremorine. A tablet formulation comprising I is given.

**IT** 131969-13-6P 131969-15-8P 131969-17-0P  
 131969-19-2P 131969-21-6P 131969-23-8P  
 131969-25-0P 131969-27-2P 131969-29-4P  
 131969-31-8P 131969-33-0P 131969-35-2P  
 131969-37-4P 131969-39-6P 131969-41-0P  
 131969-43-2P 131969-45-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as stimulant of cognitive function)

**RN** 131969-13-6 CAPLUS

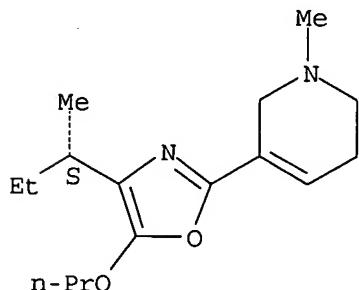
**CN** Pyridine, 1,2,3,6-tetrahydro-1-methyl-5-[4-[(1S)-1-methylpropyl]-5-propoxy-2-oxazolyl]-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131969-12-5

CMF C16 H26 N2 O2

Absolute stereochemistry.

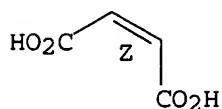


CM 2

CRN 110-16-7

CMF C4 H4 O4

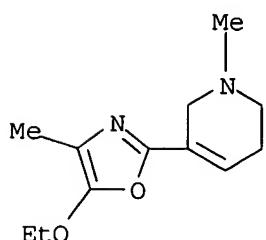
Double bond geometry as shown.



RN 131969-15-8 CAPLUS  
 CN Pyridine, 5-(5-ethoxy-4-methyl-2-oxazolyl)-1,2,3,6-tetrahydro-1-methyl-,  
 (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

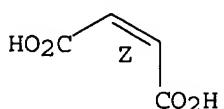
CRN 131969-14-7  
 CMF C12 H18 N2 O2



CM 2

CRN 110-16-7  
 CMF C4 H4 O4

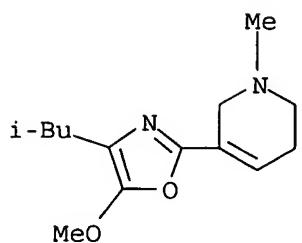
Double bond geometry as shown.



RN 131969-17-0 CAPLUS  
 CN Pyridine, 1,2,3,6-tetrahydro-5-[5-methoxy-4-(2-methylpropyl)-2-oxazolyl]-1-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

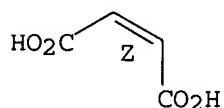
CRN 131969-16-9  
 CMF C14 H22 N2 O2



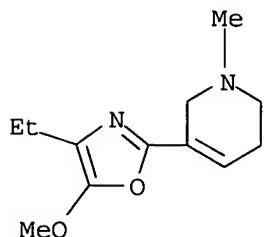
CM 2

CRN 110-16-7  
CMF C4 H4 O4

Double bond geometry as shown.

RN 131969-19-2 CAPLUS  
CN Pyridine, 5-(4-ethyl-5-methoxy-2-oxazolyl)-1,2,3,6-tetrahydro-1-methyl-,  
(2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

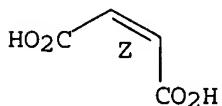
CM 1

CRN 131969-18-1  
CMF C12 H18 N2 O2

CM 2

CRN 110-16-7  
CMF C4 H4 O4

Double bond geometry as shown.



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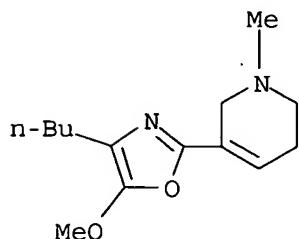
RN 131969-21-6 CAPLUS

CN Pyridine, 5-(4-butyl-5-methoxy-2-oxazolyl)-1,2,3,6-tetrahydro-1-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131969-20-5

CMF C14 H22 N2 O2

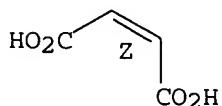


CM 2

CRN 110-16-7

CMF C4 H4 O4

Double bond geometry as shown.



RN 131969-23-8 CAPLUS

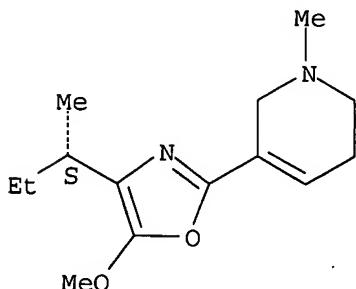
CN Pyridine, 1,2,3,6-tetrahydro-5-[5-methoxy-4-[(1S)-1-methylpropyl]-2-oxazolyl]-1-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131969-22-7

CMF C14 H22 N2 O2

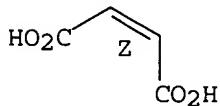
Absolute stereochemistry.



CM 2

CRN 110-16-7  
 CMF C4 H4 O4

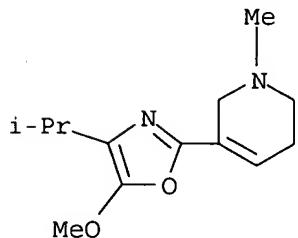
Double bond geometry as shown.



RN 131969-25-0 CAPLUS  
 CN Pyridine, 1,2,3,6-tetrahydro-5-[5-methoxy-4-(1-methylethyl)-2-oxazolyl]-1-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

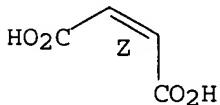
CRN 131969-24-9  
 CMF C13 H20 N2 O2



CM 2

CRN 110-16-7  
 CMF C4 H4 O4

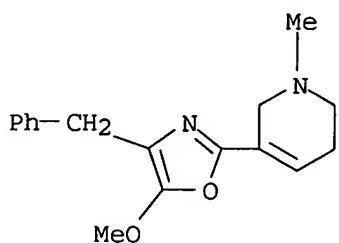
Double bond geometry as shown.



RN 131969-27-2 CAPLUS  
 CN Pyridine, 1,2,3,6-tetrahydro-5-[5-methoxy-4-(phenylmethyl)-2-oxazolyl]-1-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

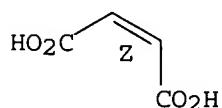
CRN 131969-26-1  
 CMF C17 H20 N2 O2



CM 2

CRN 110-16-7  
CMF C4 H4 O4

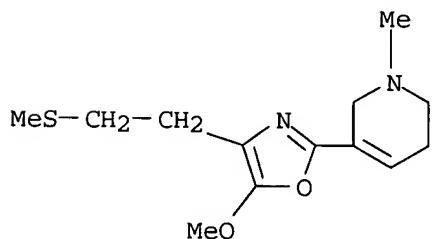
Double bond geometry as shown.



RN 131969-29-4 CAPLUS

CN Pyridine, 1,2,3,6-tetrahydro-5-[5-methoxy-4-[(2-methylthio)ethyl]-2-oxazolyl]-1-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

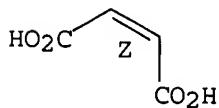
CM 1

CRN 131969-28-3  
CMF C13 H20 N2 O2 S

CM 2

CRN 110-16-7  
CMF C4 H4 O4

Double bond geometry as shown.



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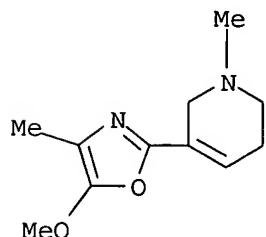
RN 131969-31-8 CAPLUS

CN Pyridine, 1,2,3,6-tetrahydro-5-(5-methoxy-4-methyl-2-oxazolyl)-1-methyl-,  
(2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131969-30-7

CMF C11 H16 N2 O2

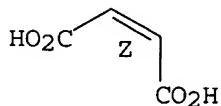


CM 2

CRN 110-16-7

CMF C4 H4 O4

Double bond geometry as shown.



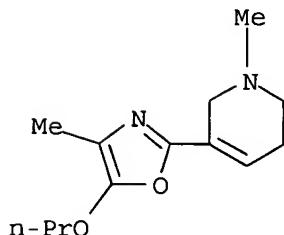
RN 131969-33-0 CAPLUS

CN Pyridine, 1,2,3,6-tetrahydro-1-methyl-5-(4-methyl-5-propoxy-2-oxazolyl)-,  
(2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131969-32-9

CMF C13 H20 N2 O2

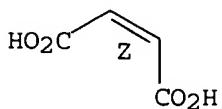


CM 2

CRN 110-16-7

CMF C4 H4 O4

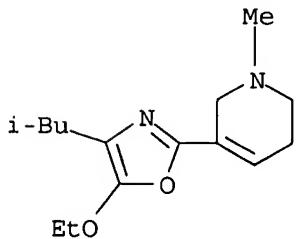
Double bond geometry as shown.



RN 131969-35-2 CAPLUS  
 CN Pyridine, 3-[5-ethoxy-4-(2-methylpropyl)-2-oxazolyl]-1,2,5,6-tetrahydro-1-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

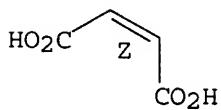
CRN 131969-34-1  
 CMF C15 H24 N2 O2



CM 2

CRN 110-16-7  
 CMF C4 H4 O4

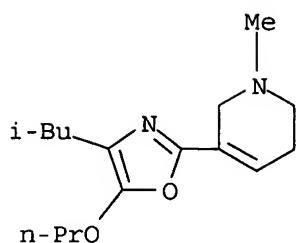
Double bond geometry as shown.



RN 131969-37-4 CAPLUS  
 CN Pyridine, 1,2,3,6-tetrahydro-1-methyl-5-[4-(2-methylpropyl)-5-propoxy-2-oxazolyl]-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

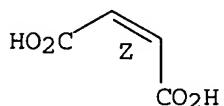
CRN 131969-36-3  
 CMF C16 H26 N2 O2



CM 2

CRN 110-16-7  
CMF C4 H4 O4

Double bond geometry as shown.



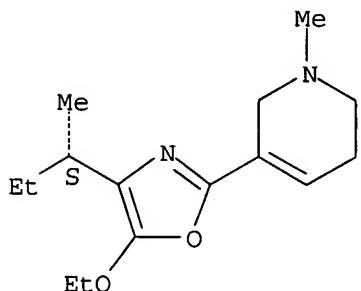
RN 131969-39-6 CAPLUS

CN Pyridine, 3-[5-ethoxy-4-[(1S)-1-methylpropyl]-2-oxazolyl]-1,2,5,6-tetrahydro-1-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131969-38-5  
CMF C15 H24 N2 O2

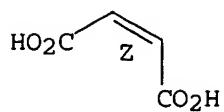
Absolute stereochemistry.



CM 2

CRN 110-16-7  
CMF C4 H4 O4

Double bond geometry as shown.



RN 131969-41-0 CAPLUS

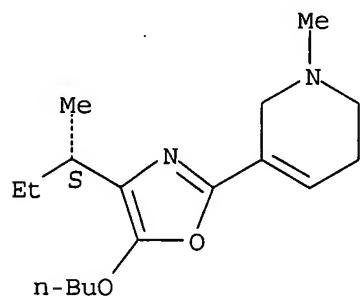
CN Pyridine, 3-[5-butoxy-4-[(1S)-1-methylpropyl]-2-oxazolyl]-1,2,5,6-tetrahydro-1-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131969-40-9

CMF C17 H28 N2 O2

Absolute stereochemistry.

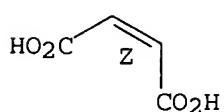


CM 2

CRN 110-16-7

CMF C4 H4 O4

Double bond geometry as shown.



RN 131969-43-2 CAPLUS

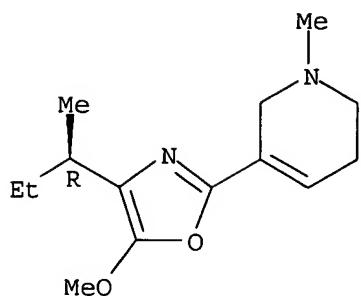
CN Pyridine, 1,2,3,6-tetrahydro-5-[5-methoxy-4-[(1R)-1-methylpropyl]-2-oxazolyl]-1-methyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131969-42-1

CMF C14 H22 N2 O2

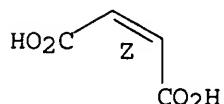
Absolute stereochemistry.



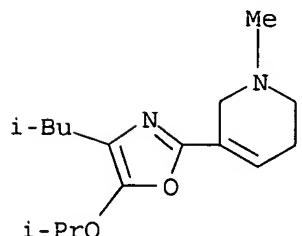
CM 2

CRN 110-16-7  
CMF C4 H4 O4

Double bond geometry as shown.

RN 131969-45-4 CAPLUS  
CN Pyridine, 1,2,3,6-tetrahydro-1-methyl-5-[5-(1-methylethoxy)-4-(2-methylpropyl)-2-oxazolyl]-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

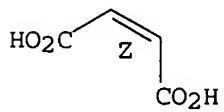
CM 1

CRN 131969-44-3  
CMF C16 H26 N2 O2

CM 2

CRN 110-16-7  
CMF C4 H4 O4

Double bond geometry as shown.



=> log Y  
COST IN U.S. DOLLARS

FULL ESTIMATED COST

	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	140.78	302.32

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-18.25	-18.25

STN INTERNATIONAL LOGOFF AT 13:18:41 ON 07 JUL 2005